Sandia National Laboratories

Development of a Platform-Independent Molecular Builder and Visualizer

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Project Description

A Unix/Linux based, platform-independent molecular builder and visualizer (MBV) was developed as a preprocessor and postprocessor for atomistic simulations. This project drew on the substantial experience and accomplishment of the VNIIEF team in this area. Developments were selected, in particular, to enable atomistic simulations of crystal defects, grain boundaries, and *material interfaces*, which are topics of active interest at Sandia and VNIIEF and in the wider materials science and solid state physics communities. Joint research was conducted to identify how to define the atomistic configurations of material interfaces in the geometric (unrelaxed) approximation, which include both grain boundaries and heterogeneous *material interfaces*. Specific capabilities for constructing grain boundaries and *material interfaces* were then implemented in the MBV. The resulting capability is being deployed at both labs to enhance productivity of analyses and investigations with atomistic methods.

Eight of nine contracted tasks have been performed to date. Highlights of the MBV capabilities are as follows:

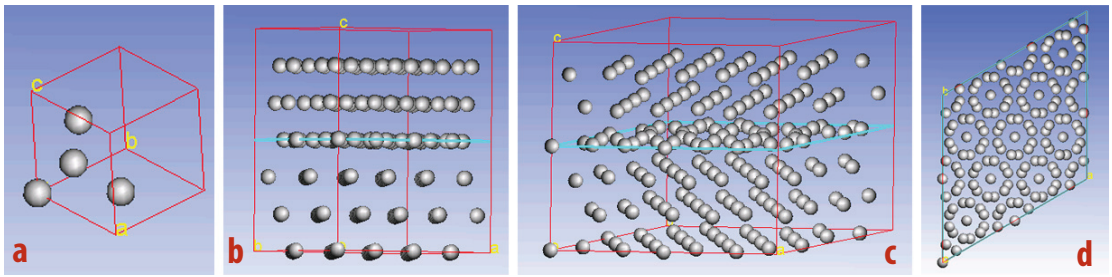
The basic, GUI-driven capability supports construction of single crystal atomistic configurations of any space group symmetry with the option of specifying a super cell for the simulation by replicating the unit cell. Included in this is the ability to easily modify the atom configurations, locally, to output several formats, and to visualize results from a variety of atomistic simulation codes. Additional modules include the capability to cleave a bulk crystal and to add molecules or atoms onto the cleaved surface; to construct grain boundary (GB) configurations that form commensurate interfaces, in the geometric (unrelaxed) approximation; to construct an arbitrary bi-crystal slab material interface structure composed of atoms or molecules of the user's choice and having periodic boundary conditions (PBCs) in two orthogonal directions in the plane of the interface. Bi-crystal and material interface configuration can each be altered by interactively selecting and shifting, removing, or adding particular atoms.

Under development is the capability to build supercells of crystals with polyatomic unit cell bases. The specific aim is to enable construction of molecular solids.

Delivered with each task are the MBV software, installation procedure instructions, and the updated Users' Manual.

The capability to construct material interfaces is fairly general, though constrained by the requirement that the resulting systems admit periodic boundary conditions in the directions in the plane of the interface. The capability comprises:

- Enumeration of the symmetrical tilt GBs;
- Enumeration of the symmetrical twist GBs;
- The possibility to remove atoms closer than a specified distance from boundary plane;
- The ability to specify the width of crystals on either side of boundary plane;
- User specification of translations on either side of the interface;
- The ability to manipulate atoms to add impurities or create defects;
- The ability to apply labels to surface layer portions of atoms;
- The ability to choose 2D or 3D periodic conditions.



Example of grain boundary (GB) construction: symmetric twist GB in aluminum. (a) Aluminum unit cell. (b)-(d) Three projections of the symmetrical twist grain boundary with angle θ = 81,78680, Plane (111) and planar ∑=7.

Technical Purpose and Benefits

Molecular builders and visualizers are an enabling technology for atomistic simulation methods. They can substantially increase a materials researcher's productivity in performing atomistic numerical simulations. A number of commercial products are available, but an MBV that can be readily modified, is platform independent, and is freely available to computational scientists at DOE laboratories and other government research laboratories is highly desirable. The MBV produced in the present project also includes an efficient and easy to use graphical user interface (GUI) to enable local modifications of the atomic structures. Moreover, it has a unique capability to construct (unrelaxed) grain boundaries and material interfaces, as illustrated in the table and figure. Such configurations are the needed starting point for investigating the challenging questions of how material microstructure influences material properties and how processing details determine microstructure. These investigations are important contributors toward the long term goal of *designing* materials to have specified properties to meet NNSA mission needs.

In the near term follow-on tasks, we will transition toward using the MBV to facilitate particular computational materials research endeavors while still adding to the MBV capabilities and providing for any needed maintenance or bug fixes to the utility. The chosen research topic is the response of molecular crystals to shock wave loading. This basic science area is of interest to RusAtom and NNSA laboratories for its relevance to high explosive safety.

Visualizers / Futures	MolDraw	ACD/Structure Drawing Applet	MW3D Crystal Lab	Crystal Studio	Crystal Maker	CaRIne Crystallography	MBV
Platform, OS	Windows	Multiplatform	Multiplatform	Windows	Windows XP Mac OS	Windows Linux	Multiplatform
3D visualization (OpenGL)	–	–	+	+	+	+	+
3D Tools (zoom, rotation…)	+	–	+	+	+	+	+
Geometrical Tools	+	+	–	+	+	+	+
Lattice builder	+	–	–	+	+	+	+
Simulation/ Animation	+/–	– /–	– /–	+/+	+/+	+/+	+/+
Surface cleaving	–	–	–	+	–	+	+
RDF/ MSD/ Temperature calc.	–/–/–	–/–/ –	–/–/ –	–/–/ –	–/–/ –	+/–/ –	+/+/+
Multi-windows support	–	–	–	+	+	+	+
X-Ray diffraction patterns	–	–	–	+	–	+	–
Defects, dislocations	–	–	–	+	+	+	+
Surface builder	–	–	–	+	–	+	+
GB Construction	–	–	–	–	–	–	+
Export formats	Gaussian, CRYSTAL 98, GULP, EXAFS, MOLPLOT, Phio-78, PLUTON, Shakal, XMOL, POV-Ray	MDL molfile	PDB	CIF, CSV, XYZ, XRD, POV-Ray	CCL, Chem3D, CIF, CSSR, FDAT, ICSD, PDB, SHELX, Struplo, MacMolecule	N/A	CERIUS, MOPAC, VASP, PDB, XYZ, CIF
Import formats	Gaussian, Crystal 2000, ADF, Mopac, HyperChem, XTL, EXAFS, CSD, PDB, XMOL, CIF	MDL molfile	PDB	CIF, CSV, XYZ, XRD, POV-Ray	Chem3D, CIF, PDB, MacMolecule	N/A	CERIUS, MOPAC, VASP, PDB, XYZ, CIF
Price	free	free	free	1398$	429-1899	795-5895	free

Comparison of Available Visualization Utilities.

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